PERGAMON

Applied Mathematics Letters 14 (2001) 245–252

Applied Mathematics Letters

www.elsevier.nl/locate/aml

Theoretical Foundations for Tail Electron Hydrodynamical Models in Semiconductors

A. M. ANILE AND G. MASCALI
Dipartimento di Matematica
University of Catania
Viale A. Doria 6, 95125 Catania, Italy

(Received May 1999; accepted June 1999)

Communicated by C. Cercignani

Abstract—In this article, we present a theoretical foundation for tail electron hydrodynamical models (TEHM) in semiconductors.

Keywords—Semiconductors, Boltzmann equation, Hydrodynamical models.

1. INTRODUCTION

The design of modern electron devices requires increasingly accurate physical models of carrier transport in semiconductors in order to be able to describe high-field phenomena such as hot electron effects, impact ionization, thermal self-heating, etc.

Hot electron phenomena are of particular interest for the accurate evaluation of the degradation and breakdown of devices.

Current calculations using Monte Carlo methods are extremely CPU intensive because of the need to gather enough data in order to obtain reliable statistics for the rare events involving hot electrons and, therefore, are not practical for routine design applications.

Traditional hydrodynamical models for carrier transport in semiconductors cannot describe hot electrons because they deal only with average values over the whole carrier population.

Therefore, it would be desirable to have a theoretically founded hydrodynamical-like model, computationally much simpler than Monte Carlo simulation, in which average quantities related to hot electrons would appear explicitly as field variables. Several considerations [1] lead to the possibility of treating hot electrons as a reasonably well-defined subpopulation of the whole carrier population, suggesting a hydrodynamical treatment of hot electrons in terms of density, temperature, etc.

In fact, many authors [2,3] have introduced new fluid dynamical models in which macroscopic quantities relative to the so-called tail electrons appear as new fundamental variables.

We acknowledge partial support from Italian Consiglio Nazionale delle Ricerche (Prog. N.96.03855.CT01) and from the Training and Mobility of Researchers Programme N. ERBFMRXCT970157. We also acknowledge stimulating comments from one of the referees.

0893-9659/00/$ - see front matter Typeset by $\mathcal{A}\mathcal{M}\mathcal{S}$-TEX
PII: S0893-9659(00)00144-0

For example, in the tail electron hydrodynamical model of Ahn *et al.* [2], hot electron phenomena are dominated by tail electrons having energies higher than a threshold energy and a tail electron hydrodynamic model (TEHM) is developed, by taking the moments of the tail electron transport equation and making a reasonable ansatz for the closures, based on Monte Carlo calibration.

Likewise, in the hot electron subpopulation (HES) model of Scrobohaci and Tang [3], in the moment equations the closures are achieved by assuming empirical equations obtained by fitting the Monte Carlo data to *ad hoc* equations.

On the contrary, in this paper we sought to achieve a theoretical foundation for TEHM by utilizing a closure method which allows to obtain both the constitutive fluxes and the production terms as functions of the fundamental hydrodynamical variables without resorting to M.C. simulations.

2. BOLTZMANN TRANSPORT EQUATION AND MOMENT EQUATIONS

We treat the case in which the current is due only to electrons (unipolar devices).

The electron transport in semiconductors is described by the Boltzmann transport equation (BTE) [4–6] coupled to the Poisson equation for the electric potential

$$\frac{\partial f}{\partial t} + v_i \frac{\partial f}{\partial x^i} - \frac{q\,E_i}{\hbar}\frac{\partial f}{\partial k_i} = Q(f), \tag{1}$$

$f(\mathbf{x}, t, \mathbf{k})$ is the one-particle electron distribution function with $\mathbf{k}$ electron wave vector belonging to the first Brillouin Zone B, $\mathbf{E}$ electric field, $\hbar$ reduced Planck constant, q electron charge, and

$$\mathbf{v} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon(\mathbf{k}),$$

electron group velocity which depends on the electron energy, $\epsilon(\mathbf{k})$, in the conduction band (which we assume to be unique for simplicity).

We will use the parabolic band approximation for which

$$\epsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2\,m^*}, \qquad B = \Re^3,$$

m^* being the electron effective mass.

Q is the collision operator which in the nondegenerate case has the form [5]

$$Q(f) = \int d\mathbf{k}' \left[w(\mathbf{k}, \mathbf{k}')\, f(\mathbf{k}') - w(\mathbf{k}', \mathbf{k})\, f(\mathbf{k})\right],$$

$w(\mathbf{k}, \mathbf{k}')$ representing the electron scattering rate from a state with momentum $\mathbf{k}'$ to one with momentum $\mathbf{k}$.

Introducing a threshold energy, ϵ_{thr}, for the electrons (which usually corresponds to the threshold energy of impact ionization) and the kinetic quantities $1, \mathbf{v}, \epsilon, \epsilon\,\mathbf{v}$, we consider the fundamental variables: number density, average velocity, and energy of electrons having energy less than and greater than ϵ_{thr} (Zone 1 and 2 electrons, respectively), plus the energy flux of electrons in Zone 1[1]:

$$\begin{aligned} n_1 &= \int_{\tilde\Delta} f\, d\mathbf{k}, & n_1\, \mathbf{u}_1 &= \int_{\tilde\Delta} \mathbf{v} f\, d\mathbf{k}, \\ n_1\, W_1 &= \int_{\tilde\Delta} \epsilon f\, d\mathbf{k}, & n_1\, \mathbf{S}_1 &= \int_{\tilde\Delta} \epsilon \mathbf{v} f\, d\mathbf{k}, \end{aligned} \tag{2}$$

[1]With the closure that we shall adopt for the high energy component, it will not be necessary to include also the energy flux of the high energy electrons.

$$n_2 = \int_\Delta f\, d\mathbf{k}, \qquad n_2\, \mathbf{u}_2 = \int_\Delta \mathbf{v} f\, d\mathbf{k},$$
$$n_2\, W_2 = \int_\Delta \epsilon f\, d\mathbf{k}, \tag{3}$$

with $\Delta = \{\mathbf{k} : \epsilon(\mathbf{k}) \geq \epsilon_{\text{thr}}\}$ and $\tilde{\Delta} = \Re^3 - \Delta$.

From the BTE one can obtain the following evolution equations for these macroscopic quantities:

$$\begin{aligned}
&\frac{\partial n_2}{\partial t} + \frac{\partial n_2\, u_2^i}{\partial x^i} - q\, E_i\, N^i = C_{n_2},\\
&\frac{\partial n_2\, u_2^j}{\partial t} + \frac{\partial n_2\, K_B\, T_2^{ij}}{\partial x^i} - q\, E_i\, U^{ji} + q\, E^j\, \frac{n_2}{m^*} = C_{u_2^j},\\
&\frac{\partial n_2\, W_2}{\partial t} + \frac{\partial n_2\, S_2^i}{\partial x^i} - q\, \epsilon_{\text{thr}} E^i\, N_i + q\, E_i\, n_2\, u_2^i = C_{W_2},
\end{aligned} \tag{4}$$

$$\begin{aligned}
&\frac{\partial n_1}{\partial t} + \frac{\partial n_1\, u_1^i}{\partial x^i} = C_{n_1} - q\, E_i\, N^i,\\
&\frac{\partial n_1\, u_1^j}{\partial t} + \frac{\partial n_1\, K_B\, T_1^{ij}}{\partial x^i} + q\, E^j\, \frac{n_1}{m^*} = C_{u_1^j} - q\, E_i\, U^{ji},\\
&\frac{\partial n_1\, W_1}{\partial t} + \frac{\partial n_1\, S_1^i}{\partial x^i} + q\, E_i\, n_1\, u_1^i = C_{W_1} - q\, \epsilon_{\text{thr}} E^i\, N_i,\\
&\frac{\partial n_1\, S_1^j}{\partial t} + \frac{\partial n_1\, S_1^{ij}}{\partial x^i} + q\, E_i\, n_1\, K_B\, T_1^{ij} + q\, E^j\, \frac{n_1\, W_1}{m^*} = C_{S_1^j} - q\, \epsilon_{\text{thr}} E_i\, U^{ji},
\end{aligned} \tag{5}$$

where the Einstein summation convention has been used throughout, K_B is the Boltzmann constant, and

$$\begin{aligned}
N^i &= \frac{1}{\hbar} \int_\Sigma f\, \nu^i\, d\sigma, & U^{ji} &= \frac{1}{\hbar} \int_\Sigma v^j f\, \nu^i\, d\sigma,\\
n_2\, K_B\, T_2^{ij} &= \int_\Delta v^i\, v^j\, f\, d\mathbf{k}, & n_2\, S_2^i &= \int_\Delta \epsilon\, v^i\, f\, d\mathbf{k},\\
n_1\, K_B\, T_1^{ij} &= \int_{\tilde{\Delta}} v^i\, v^j\, f\, d\mathbf{k}, & n_1\, S_1^{ij} &= \int_{\tilde{\Delta}} \epsilon\, v^i\, v^j\, f\, d\mathbf{k},
\end{aligned} \tag{6}$$

$$\begin{aligned}
C_{n_2} &= \int_\Delta Q\, d\mathbf{k}, & C_{u_2^j} &= \int_\Delta v^j Q\, d\mathbf{k}, & C_{W_2} &= \int_\Delta \epsilon Q\, d\mathbf{k},\\
C_{n_1} &= \int_{\tilde{\Delta}} Q\, d\mathbf{k}, & C_{u_1^j} &= \int_{\tilde{\Delta}} v^j Q\, d\mathbf{k}, & C_{W_1} &= \int_{\tilde{\Delta}} \epsilon Q\, d\mathbf{k}, & C_{S_1^j} &= \int_{\tilde{\Delta}} \epsilon v^j Q\, d\mathbf{k}.
\end{aligned} \tag{7}$$

with $\Sigma = \{\mathbf{k} : \epsilon(\mathbf{k}) = \epsilon_{\text{thr}}\}$, and $\boldsymbol{\nu}$ inner normal to Σ.

The first set of equations is found by integrating the BTE over Δ, while the second set is derived by subtracting the first one to the usual moment equations.

The preceding equations have the same form as those of the conventional HD model [5], except for the surface terms, N^i and U^{ij}, which represent the increasing rate of the corresponding macroscopic quantities due to the net migration of carriers from one energy zone to the other owing to the driving electric field.

The number of variables which appear in (4),(5) exceeds the number of equations, so that, in order to obtain a closed system of equations, we need to express the quantities (6),(7) as functions of the fundamental variables (2),(3), that is, we have to find *constitutive relations* for these quantities.

3. CLOSURE

The problem of obtaining constitutive equations can be tackled by making a suitable ansatz for the distribution function.

Here, in particular, we resort to an asymptotic solution of the Boltzmann equation recently found by Liotta and Majorana [7] in the high energy limit for homogeneous stationary cases, in order to find the constitutive functions relative to the electrons in Zone 2 (which seems appropriate because these electrons fall within the asymptotic zone).

This asymptotic solution for large energies suggests a dependence of the electron distribution function on the number density n_2, the average energy W_2, and velocity $\mathbf{u}_2$ of the form

$$f(\mathbf{x},t,\mathbf{k}) = \alpha(\mathbf{x},t,\epsilon(\mathbf{k})) + \beta(\mathbf{x},t,\epsilon(\mathbf{k}))\, k_i\, u_2^i(\mathbf{x},t) \tag{8}$$

with

$$\alpha(\mathbf{x},t) = \alpha_0(\mathbf{x},t)\, e^{-\epsilon(\mathbf{k})/\theta}, \qquad \beta = -\frac{3}{2}\,\frac{\hbar\, h(\theta)}{(\theta+\epsilon_{\text{thr}})}\, e^{\epsilon_{\text{thr}}/\theta}\, \epsilon^{-1/2}\, \frac{d\alpha}{d\epsilon},$$

α_0 being related to the number density n_2 through

$$\alpha_0 = \frac{\sqrt{2}\,\hbar^3\, m^{*-3/2}}{8\,\pi\, h(\theta)}\, n_2(\mathbf{x},t)$$

and

$$h(\theta) = \int_{\epsilon_{\text{thr}}}^{\infty} e^{-\epsilon/\theta}\epsilon^{1/2}\, d\epsilon = \theta\, \epsilon_{\text{thr}}^{1/2} e^{-\epsilon_{\text{thr}}/\theta} + \frac{\sqrt{\pi}}{2}\,\theta^{3/2}\ \text{erfc}\left(\sqrt{\frac{\epsilon_{\text{thr}}}{\theta}}\right)$$

where erfc is the complementary error function and θ is a variable related to W_2 by means of the invertible ($\frac{dW_2}{d\theta} > 0$, $\forall \epsilon_{\text{thr}}$) relation

$$W_2 = \frac{\theta}{h(\theta)}\, \epsilon_{\text{thr}}^{3/2}\, e^{-\epsilon_{\text{thr}}/\theta} + \frac{3}{2}\,\theta.$$

This expression is valid for $\epsilon \gg \hbar\omega_{\text{op}}$ where ω_{op} is the optical phonon frequency.

With regard to Zone 1 for want of a better alternative (due to the lack of asymptotic solutions in this energy range) we exploit the Maximum Entropy Principle (MEP) (see [8] and references therein), which amounts to closing the higher order moments by using the Maximum Entropy distribution function.

Because, in the present case, the moments describing the *cold electrons* are $n_1, \mathbf{u}_1, W_1$, and $\mathbf{S}_1$, this distribution function [9] reads:

$$f_{\text{M.E.}} = \exp\left[-\lambda - \epsilon\left(\frac{1}{\theta_L} + \lambda_w\right) - v^i\left(\lambda_i + \lambda_i^S \epsilon\right)\right] \tag{9}$$

where $\theta_L = K_B T_L$, T_L lattice temperature and the Lagrange multipliers λ's have to be expressed as functions of the known moments by substituting (9) into (2) and solving the resulting system with respect to λ's.

Actually it is not always possible to obtain an exact explicit representation of the Lagrange multipliers on the fundamental variables and, in general, one has to resort to numerical procedures or to suitable approximation methods.

Here, based on Monte Carlo results, we assume that the anisotropy of f is small [9], and expand $f_{\text{M.E.}}$ with respect to a suitable anisotropy parameter.

At first order in anisotropy, the distribution function reads

$$f_{\text{M.E.}} = e^{-\lambda^{(0)}}\, e^{-\lambda_w^{(0)}\epsilon}\left\{1 - v_i\left[(g_1+\epsilon\, d_1)\, u_1^i + (g_2 + \epsilon\, d_2)\, S_1^i\right]\right\} \tag{10}$$

where g_1, g_2, d_1, and d_2 are functions of W_1 which are reported in Appendix A, while $\lambda^{(0)}$ and $\lambda_w^{(0)}$ are expressed as functions of n_1 and W_1 by means of

$$n_1 = \frac{4\sqrt{2}\,\pi}{\hbar^3}\, m^{*3/2} C_{1/2}\, e^{-\lambda^{(0)}},$$
$$W_1 = \frac{C_{3/2}}{C_{1/2}},$$

$C_{n/2}$ being functions of $\lambda_w^{(0)}$ also reported in Appendix A.

Being $\frac{dW_1}{d\lambda_w^{(0)}} < 0$ for every value of ϵ_{thr}, the last expression can be inverted and $\lambda_w^{(0)}$ written as a function of W_1.

Now, we are in conditions to close our system of evolution equations by substituting the distribution functions (8) and (10) into the expressions (6) and (7).

For the surface terms and fluxes we obtain

$$N^i = -\frac{8\,\pi}{3\,\hbar^3}\sqrt{2\,m^*}\,\epsilon_{\text{thr}}^{3/2}\,e^{-\lambda^{(0)}-\lambda_w^{(0)}\,\epsilon_{\text{thr}}}\left[(g_1+\epsilon_{\text{thr}}\,d_1)\;u_1^i+(g_2+\epsilon_{\text{thr}}\,d_2)\;S_1^i\right],$$

$$U^{ij} = -\frac{8\,\pi}{3\,\hbar^3}\sqrt{2\,m^*}\,\epsilon_{\text{thr}}^{3/2}\,e^{-\lambda^{(0)}-\lambda_w^{(0)}\,\epsilon_{\text{thr}}}\,\delta^{ij},$$

$$K_B\,T_{1|2}^{ij} = \frac{2}{3}\,\frac{W_{1|2}}{m^*}\,\delta^{ij},\qquad S_1^{ij} = \frac{2}{3}\,m^{*-1}\,\frac{C_{5/2}}{C_{1/2}}\,\delta^{ij},\qquad S_2^i = \frac{\epsilon_{\text{thr}}^2+2\epsilon_{\text{thr}}\theta+\theta^2}{\epsilon_{\text{thr}}+\theta}\,u_2^i.$$

4. PRODUCTION TERMS

As regards the production terms, we take into consideration the interaction between electrons and nonpolar optical phonons, that between electrons and acoustical phonons in its elastic approximation (valid when the thermal energy is much greater than that of the phonon involved in the scattering) and the scattering of electrons with impurity centers. Then the collision operator is written as the sum of two parts:

- the first part due to the phonon-electron collisions for which the transition rate reads [6]

  $$w^{\text{ph}}\,(\mathbf{k},\mathbf{k}') = \mathcal{K}_{\text{op}}\left[n_{\text{op}}\,\delta\,(\epsilon-\epsilon'-\hbar\omega_{\text{op}})+(n_{\text{op}}+1)\delta\,(\epsilon-\epsilon'+\hbar\omega_{\text{op}})\right]+\mathcal{K}_{\text{ac}}\,\delta\,(\epsilon-\epsilon')\,,$$

  where $\mathcal{K}_{\text{op}}$ and $\mathcal{K}_{\text{ac}}$ are, respectively, the nonpolar optical and acoustical scattering kernel coefficients, assumed constant at a first approximation, n_{op} is the thermal equilibrium optical phonon number;
- the second part relative to the impurity-electron interaction which, in the Grinberg-Luryi approximation [10] (giving the same results as the exact operator for distribution functions which are only slightly anisotropic as in our case) can be written in the form

  $$Q_{\text{imp}}(f) = -\frac{f(\mathbf{k})-f_0(\epsilon(\mathbf{k}))}{\tau_{\text{imp}}(\epsilon(\mathbf{k}))},$$

  where f_0 is the isotropic part of the distribution function, and τ_{imp}, the scattering time due to interactions with impurities of charge $Z\,q$, is such that

  $$\frac{1}{\tau_{\text{imp}}} = \frac{\pi}{2}\,\frac{\hbar\,k}{m^*}\,\frac{q^4\,Z^2\,N_{\text{imp}}}{\epsilon_0^2\,\epsilon^2(\mathbf{k})}\left[\ln\left(\frac{8\,m^*\,\epsilon(\mathbf{k})+\hbar^2\,\kappa^2}{\hbar^2\,\kappa^2}\right)+\frac{8\,m^*\,\epsilon(\mathbf{k})}{8\,m^*\,\epsilon(\mathbf{k})+\hbar^2\,\kappa^2}\right]$$

  with N_{imp} concentration of impurity centers, ϵ_0 dielectric permittivity, and κ inverse screening length.

The results for the production terms (7) are reported in Appendix B.

5. CONCLUSIONS

As a test for the model we propose (being inappropriate a comparison with the models of [2,3], where a nonparabolic energy band for the conduction electrons is used), we have calculated the electron average velocity in stationary regime for different values of the external electric field by numerically solving the equations (4),(5) in the case of homogeneous bulk silicon.

In Figure 1, our results are compared to those obtained by means of a one-fluid model with the maximum entropy closure and those found in the kinetic approach by Liotta and Majorana.

For strong electric fields at which the *hot electrons* become relevant, our results are closer to those derived in the kinetic framework of Liotta and Majorana than those found by means of the one-fluid model.

More extended results, including the consideration of a nonparabolic energy band and, therefore, comparisons to the models of [2,3], will be presented in a future work which is in progress.

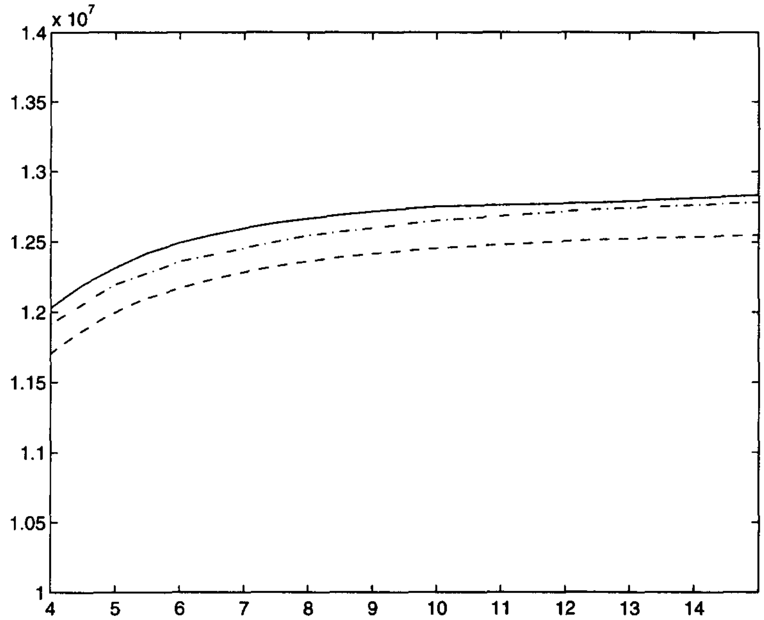

Figure 1. Velocity (cm/s) vs. electric field (V/μm). Continuous line: Kinetic model. Dashed-dotted line: two-fluid model. Dashed line: one-fluid model. $\epsilon_{\text{thr}} = 0.605\,\text{eV}$.

APPENDIX A

The functions g_1, g_2, d_1, and d_2 are given by

$$\begin{aligned} g_1 &= \frac{3}{2} m^* \lambda_w^{(0)} d \left[2\,\xi^{1/2} e^{-\xi} \left(8\,\xi^3 + 28\,\xi^2 + 70\,\xi + 105\right) - 105\sqrt{\pi}\,\text{erf}\left(\xi^{1/2}\right)\right] \left[\sqrt{\pi}\,\text{erf}\left(\xi^{1/2}\right)\right. \\ &\quad \left. -2\,e^{-\xi}\sqrt{\xi}\right], \\ g_2 &= 3\,m^* \lambda_w^{(0)2} d \left[15\sqrt{\pi}\,\text{erf}\left(\xi^{1/2}\right) - 2\,\xi^{1/2} e^{-\xi}\left(4\,\xi^2 + 10\,\xi + 15\right)\right] \left[\sqrt{\pi}\,\text{erf}\left(\xi^{1/2}\right)\right. \\ &\quad \left. -2\,e^{-\xi}\sqrt{\xi}\right], \\ d_1 &= g_2, \\ d_2 &= -6\,m^* \lambda_w^{(0)3} d \left[3\sqrt{\pi}\,\text{erf}\left(\xi^{1/2}\right) - 2\,\xi^{1/2} e^{-\xi}\left(2\,\xi + 3\right)\right] \left[\sqrt{\pi}\,\text{erf}\left(\xi^{1/2}\right) - 2\,e^{-\xi}\sqrt{\xi}\right], \end{aligned}$$

where

$$\begin{aligned} \xi &= \lambda_w^{(0)} \epsilon_{\text{thr}}, \\ d &= \left[4\,e^{-2\,\xi}\left(2\,\xi^3 + 60\,\xi^2 + 45\,\xi\right) + 45\,\pi\,\text{erf}\left(\xi^{1/2}\right)^2\right. \\ &\quad \left. +12\sqrt{\pi}\,\text{erf}\left(\xi^{1/2}\right) e^{-\xi}\,\xi^{1/2}\left(-2\,\xi^3 + 3\,\xi^2 - 10\,\xi - 15\right)\right]^{-1}. \end{aligned}$$

And for $n = 2\,m + 1$

$$C_{n/2} = (-)^m \frac{d^m}{d\,\lambda_w^{(0)\,m}} \left\{ -\lambda_w^{(0)\,-1} e^{-\lambda_w^{(0)} \epsilon_{\text{thr}}} \epsilon_{\text{thr}}^{1/2} + \frac{\sqrt{\pi}}{2} \lambda_w^{(0)-3/2}\,\text{erf}\left(\sqrt{\lambda_w^{(0)} \epsilon_{\text{thr}}}\right)\right\},$$

erf is the error function.

APPENDIX B

In this appendix, we report the results for the production terms

$$C_{n_2} = \frac{4\,\pi\sqrt{2}\,m^{*3/2}}{\hbar^3\,h(\theta)} \mathcal{K}_{\text{op}}\, n_2\, n_{\text{op}}\, \gamma_1^+\left(\epsilon_{\text{thr}}^-, \epsilon_{\text{thr}}\right)\left\{1 - e^{\hbar\omega_{\text{op}}/\theta_L - \hbar\omega_{\text{op}}/\theta}\right\},$$

$$
\begin{aligned}
C_{\mathbf{u}_2} = & -\frac{4\,\pi\,\sqrt{2}}{\hbar^3}\,\frac{m^{*3/2}\,e^{\epsilon_{\rm thr}/\theta}}{\theta(\theta+\epsilon_{\rm thr})}\,\mathcal{K}_{\rm op}\,n_2\mathbf{u}_2\left\{n_{\rm op}\left[e^{\hbar\omega_{\rm op}/\theta_L}\left(\gamma_2^-\left(\epsilon_{\rm thr},\epsilon_{\rm thr}^+\right)+\gamma_2^-\left(\epsilon_{\rm thr}^+,\infty\right)\right)\right.\right. \\
& \left.\left. +\ \gamma_2^+(\epsilon_{\rm thr},\infty)\right]+\mathcal{K}\,\theta\left[\frac{3}{2}\,h(\theta)+\epsilon_{\rm thr}^{3/2}e^{-\epsilon_{\rm thr}/\theta}\right]\right\}-\frac{\pi}{\sqrt{2\,m^*}}\,\frac{q^4Z^2N_{\rm imp}}{\epsilon_0^2\theta(\theta+\epsilon_{\rm thr})}\,e^{\epsilon_{\rm thr}\theta}G_1\,n_2\mathbf{u}_2, \\
C_{W_2} = & \ \frac{4,\pi\,\sqrt{2}}{\hbar^3}\,\frac{m^{*3/2}\,n_2}{h(\theta)}\,\mathcal{K}_{\rm op}\,n_{\rm op}\,\left\{\gamma_1^+(\epsilon_{\rm thr},\infty)\,\hbar\omega_{\rm op}\left[1-e^{\hbar\omega_{\rm op}/\theta_L-\hbar\omega_{\rm op}/\theta}\right]\right. \\
& \left. +\ \gamma_1^{-(1)}\left(\epsilon_{\rm thr},\epsilon_{\rm thr}^+\right)\,\left[e^{\hbar\omega_{\rm op}/\theta}-e^{\hbar\omega_{\rm op}/\theta_L}\right]\right\}, \\
C_{n_1} = & -C_{n_2}, \\
C_{\mathbf{u}_1} = & \ \frac{(8\,\pi)^2}{3\,\hbar^6}\,m^{*2}\,e^{-\lambda^{(0)}}\,\mathcal{K}_{\rm op}\left\{\mathbf{S}_1\left[n_{\rm op}\,\left(\zeta_1^{(1)}\,g_2+\zeta_1^{(2)}\,d_2\right)+\mathcal{K}\left(\eta^{(2)}\,g_2+\eta^{(3)}\,d_2\right)\right.\right. \\
& +\ (n_{\rm op}+1)\,\left.\left(\zeta_2^{(1)}\,g_2+\zeta_2^{(2)}\,d_2\right)\right]+\mathbf{u}_1\left[n_{\rm op}\,\left(\zeta_1^{(1)}\,g_1+\zeta_1^{(2)}\,d_1\right)+\mathcal{K}\left(\eta^{(2)}\,g_1+\eta^{(3)}d_1\right)\right. \\
& \left.\left. +\,(n_{\rm op}+1)\left(\zeta_2^{(1)}g_1+\zeta_2^{(2)}d_1\right)\right]\right\}-\frac{8\pi m^{*3/2}}{\sqrt{2}\,\hbar^3\,\theta}\,\mathcal{K}_{\rm op}\,n_{\rm op}\,\frac{n_2\,\mathbf{u}_2}{\theta+\epsilon_{\rm thr}}\,e^{\epsilon_{\rm thr}/\theta}\,\gamma_2^+\left(\epsilon_{\rm thr}^-,\epsilon_{\rm thr}\right) \\
& +\ \frac{8\,\pi^2}{3\,\hbar^3}\,\frac{N_{\rm imp}\,q^4\,Z^2}{\epsilon_0^2}\,e^{-\lambda^{(0)}}\,\left[\mathbf{S}_1\left(G_2^{(0)}\,g_2+G_2^{(1)}\,d_2\right)+\mathbf{u}_1\left(G_2^{(0)}\,g_1+G_2^{(1)}\,d_1\right)\right], \\
C_{W_1} = & \ \frac{4\,\pi}{\hbar^3}\,m^{*3/2}\mathcal{K}_{\rm op}\left\{\frac{\sqrt{2}\,n_2}{h(\theta)}\,\gamma_1^{+(1)}\left(\epsilon_{\rm thr}^-,\epsilon_{\rm thr}\right)\,n_{\rm op}\left[e^{\hbar\omega_{\rm op}/\theta_L-\hbar\,\omega_{\rm op}/\theta}-1\right]\right. \\
& \left. +\ \frac{8\,\pi}{\hbar^3}\,m^{*3/2}\,e^{-\lambda^{(0)}}\,\hbar\omega_{\rm op}\,n_{\rm op}\,\left[\zeta_1-e^{\hbar\omega_{\rm op}/\theta_L}\,\zeta_2\right]\right\}.
\end{aligned}
$$

$C_{\mathbf{S}_1}$ is the same as $C_{\mathbf{u}_1}$ with $\zeta_{1|2}^{(n)}$, $\eta^{(n)}$, $\gamma_2^+(\epsilon_{\rm thr}^-,\epsilon_{\rm thr})$, and $G_2^{(n)}$ replaced by $\zeta_{1|2}^{(n+1)}$, $\eta^{(n+1)}$, $\gamma_2^{+(1)}(\epsilon_{\rm thr}^-,\epsilon_{\rm thr})$, and $G_2^{(n+1)}$, respectively, and

$$
\begin{aligned}
\gamma_1^{\pm(n)}(W_2;a,b) &= (-)^n\,\frac{d^n}{d(1/\theta)^n}\,\int_a^b\,\sqrt{x^2\pm\hbar\omega_{\rm op}\,x}\,e^{-x/\theta}\,dx, \\
\gamma_2^{\pm(n)}(W_2;a,b) &= (-)^n\,\frac{d^n}{d(1/\theta)^n}\,\int_a^b\,x\,\sqrt{x\pm\hbar\omega_{\rm op}}\,e^{-x/\theta}\,dx, \\
\zeta_1^{(n)}\,(W_1) &= (-)^n\,\frac{d^n}{d\,\lambda_w^{(0)\,n}}\,\left\{\int_0^{\epsilon_{\rm thr}^-}\,e^{-\lambda_w^{(0)}\,\epsilon}\,\epsilon^{1/2}\,(\epsilon+\hbar\omega_{\rm op})^{1/2}\right\}\,d\epsilon, \\
\zeta_2^{(n)} &= (-)^n\,\frac{d^n}{d\,\lambda_w^{(0)\,n}}\,\left\{e^{-\lambda_w^{(0)}\,\hbar\omega_{\rm op}}\,\zeta_1\right\}, \qquad \text{with } n=0,1,\ldots, \\
\eta^{(n)}\,(W_1) &= (-)^n\,\frac{d^n}{d\,\lambda_w^{(0)\,n}}\,\left[-\lambda_w^{(0)-1}\,e^{-\lambda_w^{(0)}\,\epsilon_{\rm thr}}+\lambda_w^{(0)-1}\right]. \\
G_1(W_2) &= \int_{\epsilon_{\rm thr}}^\infty\,\epsilon^{-1/2}\,e^{-\epsilon/\theta}\left[\ln\left(\frac{8\,m^*\,\epsilon+\hbar^2\,\kappa^2}{\hbar^2\,\kappa^2}\right)+\frac{8\,m^*\,\epsilon}{8\,m^*\,\epsilon+\hbar^2\,\kappa^2}\right]\,d\epsilon, \\
G_2^{(n)}(W_1) &= \frac{(-)^n\,d^n}{d\,\lambda_w^{(0)\,n}}\,\int_0^{\epsilon_{\rm thr}}\,e^{-\lambda_w^{(0)}\,\epsilon}\,\left[\ln\left(\frac{8\,m^*\,\epsilon+\hbar^2\,\kappa^2}{\hbar^2\,\kappa^2}\right)+\frac{8\,m^*\,\epsilon}{8\,m^*\,\epsilon+\hbar^2\,\kappa^2}\right]\,d\epsilon, \\
\epsilon_{\rm thr}^+ &= \epsilon_{\rm thr}+\hbar\omega_{\rm op}, \qquad \epsilon_{\rm thr}^-=\epsilon_{\rm thr}-\hbar\omega_{\rm op}, \quad \text{and} \quad \mathcal{K}=\frac{\mathcal{K}_{\rm ac}}{\mathcal{K}_{\rm op}}.
\end{aligned}
$$

REFERENCES

1. S. Laux and M. Fischetti, Transport models for advanced device simulation—truth or consequences. *Proceedings of the Bipolar-BiCMOS Technology Meeting*, October 1–3, Minneapolis, MN, (1995).
2. C.-S. Yao, J.-G. Ahn, Y.-J. Park, H.-S. Min and R.W. Dutton, Formulation of a tail electron hydrodynamic model based on Monte Carlo simulations, *IEEE Electron Dev. Lett.* **16**, 26–29, (1995).
3. P. Scrobohaci and T.-W. Tang, Modeling of the hot electron subpopulation and its application to the impact ionization in silicon submicron devices: Part I, *IEEE Trans. Electron Devices* **41**, 1197–1205, (1996).

4. C. Cercignani, The Boltzmann equation and its applications, *Applied Mathematical Sciences 67*, Springer-Verlag, New York, (1998).
5. A. Markowich, C.A. Ringhofer and C. Schmeiser, *Semiconductor Equations*, Springer-Verlag, Wien, (1990).
6. C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*, Springer-Verlag, New York, (1989).
7. S.F. Liotta and A. Majorana, A novel approach to spherical-harmonics expansion for electron transport in semiconductors, Preprint, University of Catania, available at this URL: `http://arXiv.org/abs/cond-mat/0003456`, (1999).
8. C.D. Levermore, Moment closure hierarchies for kinetic theories, *J. Stat. Phys.* **83**, 1021–1065, (1996).
9. A.M. Anile and V. Romano, Non parabolic band transport in semiconductors: Closure of the moment equations, *Phys. Rev. B.*, (submitted).
10. A.A. Grinberg and S. Luryi, Diffusion in a short base, *Solid-St. Electron.* **35**, 1299–1309, (1992).